

Saving the Coherent State Path Integral

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By returning to the underlying discrete time formalism, we relate spurious results in coherent state path integral calculations to the high frequency structure of their propagators. We show how to modify the standard expressions for thermodynamic quantities to yield correct results. These expressions are relevant to a broad range of physical problems, from the thermodynamics of Bose lattice gases to the dynamics of spin systems.

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Path integrals convert the difficult problem of diagonalizing a Hamiltonian into the potentially simpler one of summing over a set of all possible paths, weighted by the classical action [1, 2]. They are particularly powerful for making semiclassical approximations, where only a few classical paths dominate. Often the natural variables for describing the path are conjugate. For example, one would like to describe a spin system in terms of paths on the Bloch sphere, even though the different components of spin do not commute [3]. Coherent states are often used in such cases, and can yield useful results [4, 5]. Here, we analyze the structure of such path integrals, demonstrating a practical scheme for eliminating anomalies which were first confronted in the 1980s [6–9].

The issues we address were most clearly described by Wilson and Galitsky [10], who used two simple examples to illustrate the anomalies. For example, they consider a path integral calculation of the partition function Z'_{ss} of the single site Bose Hubbard model, $\hat{H}_{ss} = \frac{U}{2}\hat{n}(\hat{n}-1) - \mu\hat{n}$, where $\hat{n} = \hat{a}^\dagger\hat{a}$ represents the number of Bosons, U parameterizes their interaction and μ is the chemical potential. This is a sufficiently simple problem that one can calculate the exact partition function Z_{ss} , and find $Z_{ss} \neq Z'_{ss}$. In particular, at zero temperature, the mean occupation number calculated from Z'_{ss} is $\langle n' \rangle = \left[\left[\frac{\mu}{U}\right]\right]$, which the exact result derived from Z_{ss} is $\langle n \rangle = \left[\left[\frac{\mu}{U} + \frac{1}{2}\right]\right]$. Here $\left[\left[x\right]\right]$ is the integer closest to x .

We derive an algorithm for correcting the path integral result for the free energy $F = -\frac{1}{\beta} \log Z$,

$$F = F^{CPI} - i \frac{1}{4\Delta t} \int_0^\pi d\chi e^{i\chi} \log \left[\frac{\det G_{\omega=\frac{\pi}{\Delta t}e^{i\chi}}^{-1}}{2\pi} \right] \quad (1)$$

Here, $F^{CPI} = F_0 - i \sum \text{Res} \left[\frac{1}{2} \log \left[\frac{\det G_\omega^{-1}}{2\pi} \right] (e^{i\beta\omega} - 1)^{-1} \right]$ includes the classical path term F_0 and a sum of residues over the poles of $\log [\det G_\omega^{-1}]$ which generally corresponds to the quadratic corrections to the free energy obtained from the continuous-time path integral, and $[G_\omega]_{ij} = \langle \psi_\omega^i \psi_{-\omega}^j \rangle$ is the matrix of perturbation field propagators in frequency space. We precisely define all these terms below as we derive Eq. (1) and discuss techniques for calculating the correction terms.

As emphasized by Wilson and Galitsky, our corrections are not related to ambiguities of operator ordering

or geometric phases. Rather, they arise from the over-completeness of coherent states.

The formulation of partition function as a path integral in imaginary time involves the expansion

$$\begin{aligned} Z &= \text{Tr} e^{-\beta \hat{H}} = \sum_{\Psi_0} \langle \Psi_0 | e^{-\beta \hat{H}} | \Psi_0 \rangle \\ &= \sum_{\Psi_1, \dots, \Psi_{N_t}} \prod_{t=1}^{N_t} \langle \Psi_{t-1} | e^{-\hat{H} \Delta t} | \Psi_t \rangle. \end{aligned} \quad (2)$$

Here $\beta = 1/T$ is the inverse temperature. $\{|\Psi_t\rangle\}$ is any complete basis of the states, characterized by a set of parameters Ψ_t , e.g. $\Psi_t = (n, \varphi)$ so that $\hat{a}|(n, \varphi)\rangle = \sqrt{n}e^{i\varphi}|(n, \varphi)\rangle$ in the coherent state basis of the Bose-Hubbard model. The sum $\sum_{\Psi_t} |\Psi_t\rangle \langle \Psi_t| = \mathcal{I}$ is the identity operator, of which we insert $N_t - 1 \equiv \beta/\Delta t - 1$ copies into the operator. We are now summing over all N_t -point paths in Ψ -space, with $\Psi_0 = \Psi_{N_t}$. In the limit of small Δt one can approximate $e^{-\hat{H} \Delta t} \approx 1 - \hat{H} \Delta t$ and thus write the partition function in the form of a discrete time path integral $Z = \int \mathcal{D}\Psi e^{-\sum_t L_t}$, where the Lagrangian is

$$L_t = -\log [\langle \Psi_t | \Psi_{t+1} \rangle] + \Delta t \frac{\langle \Psi_t | \hat{H} | \Psi_{t+1} \rangle}{\langle \Psi_t | \Psi_{t+1} \rangle}. \quad (3)$$

When the basis $\{|\Psi\rangle\}$ is orthogonal, the first term in this expansion can be taken to be arbitrarily small, and one can approximate $|\Psi_{t+1}\rangle \approx (1 + \Delta t \partial_t)|\Psi_t\rangle$, and by taking $\Delta t \rightarrow 0$ convert the problem into the traditional continuous form [4]. This approximation breaks down when expanding in an overcomplete basis, if the overlap between consecutive time steps remains finite for states that differ to a non-infinitesimal degree.

As was previously noted [9], even in the face of this problem, the discrete time formulation in Eq. (3) remains valid. Our task is to develop a techniques for calculations using the discrete time path integrals, and to relate them to the more familiar continuous case. In particular we wish to find a correction of the form Eq. (1).

To do so we follow standard procedure and characterize the states in terms of a saddle point solution $\bar{\Psi}$ satisfying $\left[\frac{\delta L_t}{\delta \Psi_t}\right]_{\Psi_t=\bar{\Psi}} = 0$, and a fluctuation ψ_t , writing

$\Psi_t = \bar{\Psi} + \psi_t$. We then expand to quadratic order in the fluctuations $L_t = L_0 + \psi_t \cdot L_2 \cdot \psi_t + \psi_t \cdot L_{2\Delta} \cdot \psi_{t+1} + O(|\psi_t|)^3$ where the classical energy L_0 and matrices $L_2, L_{2\Delta}$ are independent of time. In terms of the Fourier components $\psi_\omega = \frac{1}{\sqrt{N_t}} \sum_t e^{-i\omega t} \psi_t$, the partition function reads

$$Z = \int \mathcal{D}\psi \exp \left[-\beta F_0 - \frac{1}{2} \sum_{\omega=\omega_n} \psi_\omega \cdot G_\omega^{-1} \cdot \psi_\omega \right] \quad (4)$$

where summation is over the frequencies $\omega_n = \frac{2\pi}{\beta} n$ for $n = \frac{N_t-1}{2} \dots \frac{N_t-1}{2}$, yielding the free energy

$$F = F_0 + \frac{1}{\beta} \sum_{\omega=\omega_n} \frac{1}{2} \log \left[\frac{\det G_\omega^{-1}}{2\pi} \right]. \quad (5)$$

While Eq. (5) has the same form as one finds in the continuous time formalism, the propagators G_ω are somewhat different, and the sum is over only a finite set of frequencies. Despite these differences, one can follow the standard procedure to replace the sum with a contour integral, using the identity

$$\begin{aligned} \frac{1}{2\pi} \oint_\gamma d\omega \frac{f(\omega)}{e^{i\beta\omega} - 1} \\ = \frac{1}{\beta} \sum_{\omega=\omega_n} f(\omega) + i \sum_{\omega_f} \text{Res} \left[\frac{f(\omega)}{e^{i\beta\omega} - 1}, \omega_f \right]. \end{aligned} \quad (6)$$

Here the last sum is over the poles ω_f of $f(\omega)$ inside the contour γ , and γ is the complex circle defined by $|\omega| = \frac{2\pi}{\beta} \frac{N_t}{2} = \frac{\pi}{\Delta t}$. The notation $\text{Res}[f(\omega), \omega_f]$ refers to the residue of $f(\omega)$ at $\omega = \omega_f$ and here $f(\omega) = \frac{1}{2} \log \left[\frac{\det G_\omega^{-1}}{2\pi} \right]$. A largely unimportant subtlety is that the singularities of $f(\omega)$ are logarithmic branch points rather than poles. In practice, when one calculates thermodynamic derivatives such as $\langle n \rangle = -\frac{\partial F}{\partial \mu}$, these become poles.

In a continuous time calculation, the integral on the left-hand side of Eq. (6) vanishes as one takes $\Delta t \rightarrow 0$. This integral involves fluctuations of frequency $\omega_{\max} = \frac{\pi}{\Delta t}$, corresponding to the time scale separating consecutive time steps. When the basis $|\Psi_t\rangle$ is orthogonal these fluctuations are vanishingly small, but for an overcomplete basis they are finite, and the contour integral does not vanish. Straightforward algebra then reduces Eq. (5) to the expression in Eq. (1).

Thus, calculation of the free energy requires only the form of $\log[\det G_\omega^{-1}]$ at its singularities $\omega = \omega_f(\Delta t)$ and its value on the contour γ . We define $\omega_f = \lim_{\Delta t \rightarrow 0} \omega_f(\Delta t)$. Generically this limit is well defined, and by taking $N_t \rightarrow \infty$, the set $\{\omega_f\}$ and the behavior of

$f(\omega)$ near ω_f become arbitrarily close to what is found using continuous time. In particular, F^{CPI} in Eq. (1) corresponds to the continuous-time path integral value of F .

A clear example of this calculation is provided by the single-site Bose-Hubbard Hamiltonian. Using the coherent state basis and the field $\psi_t = (\delta n_t, \phi_t)$, the components of the quadratic Lagrangian are

$$\begin{aligned} L_0 &= \frac{1}{2} \frac{\mu^2}{U} \Delta t \\ L_2 &= \begin{pmatrix} \frac{U}{4\mu} (1 + \mu \Delta t) & 0 \\ 0 & \frac{\mu}{U} (1 - \mu \Delta t) \end{pmatrix} \\ L_{2\Delta} &= -[1 - \mu \Delta t] \begin{pmatrix} \frac{U}{4\mu} & \frac{i}{2} \\ -\frac{i}{2} & \frac{\mu}{U} \end{pmatrix} \end{aligned} \quad (7)$$

and so

$$\log[\det G_\omega^{-1}] = \log[2(1 - \cos(\omega \Delta t))(1 - \mu \Delta t)] \quad (8)$$

has its singularity at $\omega = 0$, where the continuous-time structure result holds: this expression should be contrasted with the continuous time result $\log[\det^{CPI} G_\omega^{-1}] = \log[\beta^2 \omega^2]$. As expected, the difference between the free energies simply comes from the contour integral, and $F - F^{CPI} = -\frac{\mu}{2}$ and an irrelevant constant.

The power of this approach is more readily apparent in the multisite Bose Hubbard model [11]. Consider a D -dimensional cubic lattice of N_s sites with lattice constant a_0 . There momentum is a good quantum number and one can consider $G_{\omega, \mathbf{k}}$. The large ω structure takes on the simple form

$$\log[\det G_{\omega, \mathbf{k}}^{-1}] = \log[2(1 - \cos(\omega \Delta t))(1 + \epsilon_k \Delta t)] \quad (9)$$

where $\epsilon_k = 4J \sum_{j=1}^D \sin^2(k_j a_0/2) - \mu$. By summing over the allowed momenta one finds simply,

$$F - F^{CPI} = \frac{1}{2} (\mu - 2J \times D) N_s \quad (10)$$

plus a constant. This is the same μ dependence as the single-site problem.

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